

Materials for Sustainable Energy Applications

Conversion, Storage, Transmission, and Consumption

edited by

Xavier Moya

David Muñoz-Rojas



Materials for Sustainable Energy Applications

Materials for Sustainable Energy Applications

Conversion, Storage, Transmission, and Consumption

edited by
Xavier Moya
David Muñoz-Rojas

Published by

Pan Stanford Publishing Pte. Ltd.
Penthouse Level, Suntec Tower 3
8 Temasek Boulevard
Singapore 038988

Email: editorial@panstanford.com

Web: www.panstanford.com

British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library.

**Materials for Sustainable Energy Applications: Conversion,
Storage, Transmission, and Consumption**

Copyright © 2016 Pan Stanford Publishing Pte. Ltd.

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the publisher.

For photocopying of material in this volume, please pay a copying fee through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. In this case permission to photocopy is not required from the publisher.

ISBN 978-981-4411-81-3 (Hardcover)

ISBN 978-981-4411-82-0 (eBook)

Printed in the USA

There are many things we could do to keep ourselves going: as the oil wells run dry. We have to keep our wits about us, though. We have to co-operate the whole world over and we have to work hard and *fast*.

—Isaac Asimov, 1982

About the Editors

Xavier Moya is a Royal Society University Research Fellow in the Department of Materials Science & Metallurgy at the University of Cambridge. He received his BSc and PhD in physics from the University of Barcelona in 2003 and 2008, respectively. He is interested in phase transitions in functional materials whose structural, magnetic, electrical, and thermal properties display strong coupling. His research focuses primarily on caloric materials for cooling applications and magnetoelectric materials for data storage. Dr. Moya has been a Fellow of Churchill College since 2014. He was awarded the 2009 Ramon Margalef Prize for his PhD work and the 2015 Young Researcher in Experimental Physics Prize by the Spanish Royal Society of Physics for his continuous work on multiferroic materials.

David Muñoz-Rojas received his degree in organic chemistry in 1999 and master's degree in chemical engineering (2000) from the Instituto Químico de Sarrià (IQS, Barcelona), obtaining the P. Salvador Gil, S.I. 2000 prize. He did his PhD in materials science (2004) at the Instituto de Ciencia de Materiales de Barcelona (CSIC-UAB). Thereafter, he worked as a postdoc at the Laboratoire de Réactivité et Chimie des Solides in Amiens (France), the Research Centre for Nanoscience and Nanotechnology in Barcelona, and the University of Cambridge (Device Materials Group). Dr. Muñoz-Rojas is currently a permanent CNRS researcher at the Laboratoire des Matériaux et du Génie Physique in Grenoble, France. His research focuses on using and developing cheap and scalable chemical approaches for the fabrication of novel functional materials for electronic and optoelectronic applications. In particular, he has pioneered the development of the novel spatial atomic layer deposition (SALD) technique for the deposition of active components for optoelectronic devices. He is currently further developing SALD to extend the possibilities and fields of application of this exciting technique.

Contents

Preface

xxiii

Part 1: Introduction

1. Energy in Transition	3
<i>Pedro Gómez-Romero and David Muñoz-Rojas</i>	
1.1 Introduction	4
1.2 Materials for Energy	11
1.3 How Far Ahead Is the Future?	17

Part 2: Energy Conversion

2. Materials for Photovoltaic Solar Cells	27
<i>David Muñoz-Rojas, Hongjun Liu, João Resende, Daniel Bellet, Jean-Luc Deschanvres, Vincent Consonni, and Shanting Zhang</i>	
2.1 The Physics of Solar Cells	27
2.1.1 The p-n Junction	28
2.1.2 Performance Assessment	32
2.1.3 The Shockley–Queisser Limit	35
2.1.4 Advanced Characterization	36
2.1.5 Materials Requirement: The Ideal Solar Cell	38
2.2 Types of Solar Cell	39
2.2.1 Silicon	40
2.2.1.1 Crystalline silicon solar cells	40
2.2.1.2 Si heterojunction solar cells	41
2.2.2 Gallium Arsenide	43
2.2.3 Thin Film Technologies	44
2.2.3.1 Copper indium gallium diselenide	44

2.2.3.2	Cadmium telluride	45
2.2.3.3	Amorphous Si	46
2.2.3.4	Thin film Si, nano- and micro-Si	47
2.2.4	Emerging Technologies	48
2.2.4.1	Dye sensitized solar cells	48
2.2.4.2	Organic and hybrid solar cells	49
2.2.4.3	Inorganic and ultra-low-cost cells	50
2.2.4.4	Quantum dots cells	54
2.2.4.5	Hybrid perovskite cells	57
2.2.4.6	Spectral conversion	60
2.2.4.7	Nanostructured solar cells based on zinc oxide nanowire arrays	62
2.2.5	Multijunction or Tandem Solar Cells	65
2.3	Transparent Conductive Materials	67
2.3.1	N-Type TCOs	70
2.3.2	P-Type TCOs	71
2.3.3	TCM Based on Metallic Nanowires	72
2.3.4	TCM Based on CNT and Graphene	73
2.4	Toward Low Cost, Fast and Scalable Processing	75
3.	Low-Cost Electricity Production from Sunlight: Third-Generation Photovoltaics and the Dye-Sensitized Solar Cell	93
	<i>Nadia Barbero and Frédéric Sauvage</i>	
3.1	Introduction	93
3.2	Basics of Organic Photovoltaics	95
3.3	Dye-Sensitized Solar Cell Principle	101
3.3.1	Semiconductor and Electrolyte Development for Dye-Sensitized Solar Cells	103
3.3.2	Dye Development with Molecular Engineering	108
3.3.3	Liquid Electrolyte Development Based on Solvent and Solvent-Free Formulation for Stable Devices	123

3.3.4	Current Understanding of Chemical/Photoelectrochemical Degradation Pathways	127
3.3.5	Concluding Remarks	137
4.	Thermoelectrics	155
	<i>Damien Saurel</i>	
4.1	Introduction	155
4.2	Definition	156
4.3	Applications of Thermoelectricity	157
4.3.1	Temperature Sensing – Thermocouples	157
4.3.2	Conversion	158
4.3.2.1	Maximum efficiency	161
4.3.2.2	Maximum power	163
4.3.2.3	Thermoelectric modules	164
4.3.3	Heat Pump	166
4.4	Semiclassical Theory of Thermoelectricity in Solids	168
4.4.1	Introduction	168
4.4.2	Quasi-Free Electron Model	171
4.4.3	Electron Conductivity	174
4.4.4	Thermopower	177
4.4.5	The Sommerfeld Expansion	178
4.4.6	Electrons and Holes	182
4.4.7	Multiband Contribution	183
4.4.8	Thermal Conductivity	185
4.4.9	Figure of Merit	187
4.4.9.1	Optimum chemical potential and quality factor	187
4.4.9.2	Treatment for a single band in the low temperature limit	189
4.4.9.3	Optimum band gap	192
4.5	Thermoelectric Materials	193
4.5.1	Historical Overview	193
4.5.2	Chalcogenides	196

4.5.3	Silicon and Si-Ge Alloys	197
4.5.4	PGEC Related Materials: Skutterudites, Clathrates, and Half-Heusler	198
4.5.5	Oxides	200
4.5.6	Other Materials	201
4.6	Conclusion	201
5.	Piezoelectric Conversion	205
	<i>Steven R. Anton</i>	
5.1	Introduction	206
5.1.1	Vibration Energy Harvesting Concepts	206
5.1.2	A Brief History of Piezoelectricity	209
5.2	Principles of Piezoelectric Transduction	210
5.2.1	Piezoelectric Transduction Phenomenon	210
5.2.2	Piezoelectric Material and Transducer Types	212
5.2.3	Mathematical Modeling of Piezoelectric Energy Harvesters	216
5.2.3.1	Unimorph cantilever exact analytical solution	218
5.2.3.2	Bimorph cantilever exact analytical solution for series connection of electrodes	221
5.2.3.3	Bimorph cantilever exact analytical solution for parallel connection of electrodes	222
5.2.3.4	Approximate distributed parameter solutions	223
5.2.3.5	Summary	224
5.3	Energy Conditioning Circuitry	224
5.3.1	Rectification	225
5.3.2	DC-DC Conversion	226
5.3.3	Synchronous Extraction	228
5.3.4	Impedance Matching	230
5.3.5	Summary	232

5.4	Applications of Piezoelectric Energy Harvesting	232
5.4.1	Self-Powered Sensing Systems	232
5.4.2	Biological and Wearable Energy Harvesting	236
5.4.3	Piezoelectric Harvesting in Microelectromechanical Systems	239
5.4.4	Harvesting Fluid Flow Using Piezoelectric Transduction	242
5.4.4.1	Harvesting of liquid flow	242
5.4.4.2	Harvesting air flow using windmill-style harvesters	244
5.4.4.3	Harvesting of air flow using flutter-style harvesters	245
5.4.5	Summary	248
5.5	Current Research Thrusts	248
5.5.1	Broadband and Nonlinear Harvesting	248
5.5.1.1	Broadband piezoelectric energy harvesting	249
5.5.1.2	Nonlinear piezoelectric energy harvesting	250
5.5.2	Multifunctional Harvesting	251
5.5.3	Multi-Source Energy Harvesting	253
5.5.4	Novel Piezoelectric Materials	256
5.5.4.1	Piezoelectric single crystals	256
5.5.4.2	Piezoelectric nanocomposites	258
5.5.4.3	Piezoelectret foams	260
5.5.4.4	Lead-free piezoelectrics	262
5.6	Summary and Future Visions	263
6.	Fuel cells	277
	<i>Jesús Canales-Vázquez and Juan Carlos Ruiz-Morales</i>	
6.1	Introduction	277
6.2	History	281
6.3	Types of Fuel Cells	284
6.3.1	Alkaline Fuel Cells	286

6.3.2	Polymer Electrolyte Membrane Fuel Cells	286
6.3.3	Phosphoric Acid	288
6.3.4	Molten Carbonate	288
6.3.5	Solid Oxide Fuel Cells	289
6.4	Thermodynamics	291
6.5	Fuel Cell Efficiency	294
6.5.1	Thermodynamic Efficiency	295
6.5.2	Voltaic Efficiency	296
6.5.3	Faradaic Efficiency	300
6.5.4	Heat Efficiency	300
6.6	Applications	302
6.6.1	HyFLEET-CUTE	302
6.6.2	UTSIRA	303
6.6.3	Present and Future	304
6.6.4	Last Trends in Fuel Cell Technology	304
6.6.4.1	Alkaline fuel cells	304
6.6.4.2	Phosphoric acid fuel cells	305
6.6.4.3	Polymer electrolyte membrane fuel cells	305
6.6.4.4	Molten carbonate fuel cells	306
6.6.4.5	Solid oxide fuel cells	306

Part 3: Energy Storage

7. Batteries: Fundamentals and Materials Aspects 313

Montse Casas-Cabanas and Jordi Cabana

7.1	Introduction	313
7.1.1	What Is a Battery?	313
7.1.2	Materials Aspects	319
7.1.3	Methods for Battery Testing	323
7.1.3.1	Chronopotentiometry	323
7.1.3.2	Chronoamperometry	324
7.1.3.3	Cyclic voltammetry	325
7.1.3.4	Electrochemical impedance spectroscopy	325

7.2	Rechargeable Battery Systems	325
7.2.1	Lead Acid Batteries	325
7.2.2	Alkaline Rechargeable Batteries	329
7.2.3	Lithium Rechargeable Batteries	332
7.2.3.1	From Li metal to Li-ion	332
7.2.3.2	Negative electrodes	333
7.2.3.3	Positive electrodes	336
7.2.3.4	Electrolytes	339
7.2.3.5	... and back to Li metal	340
7.3	Beyond Li-Ion: From Single to Multivalent Ion Chemistries	342
7.4	Redox Flow Batteries	343
8.	Environmentally Friendly Supercapacitors	351
	<i>Ana Karina Cuentas-Gallegos, Daniella Pacheco-Catalán, and Margarita Miranda-Hernández</i>	
8.1	Introduction	351
8.2	Energy Storage Devices	352
8.3	Supercapacitors Background	357
8.4	Charge Storage Mechanisms	360
8.4.1	The Electric Double Layer	360
8.4.1.1	Helmholtz model	361
8.4.1.2	Gouy–Chapman model	362
8.4.1.3	Stern and modern models	363
8.4.2	Pseudocapacitance Mechanism	365
8.4.2.1	Redox reactions	366
8.4.2.2	Ion electrosorption	368
8.4.2.3	Intercalation	369
8.5	Classification	370
8.5.1	Charge Storage Mechanism	372
8.5.1.1	Electric double layer capacitors	373
8.5.1.2	Pseudocapacitors	387
8.5.1.3	Conducting organic polymers	388
8.5.1.4	Transition metal oxides	394

8.5.1.5	Hybrid supercapacitors	400
8.5.1.6	Functionalized carbons	400
8.5.1.7	Nanocomposites and/or hybrid materials	404
8.5.1.8	Asymmetric assembly	410
8.5.2	Electrolyte	421
8.5.2.1	Organic electrolytes	422
8.5.2.2	Ionic liquids	422
8.5.2.3	Polymeric electrolytes	423
8.5.2.4	Aqueous electrolytes	424
8.6	Designing High-Performance Environmentally Friendly Supercapacitors	425
8.7	Characterization	430
8.7.1	Electrode Fabrication	430
8.7.2	Electrode Material Characterization	433
8.7.3	Cell Characterization	437
8.7.3.1	Cyclic voltammetry	437
8.7.3.2	Galvanostatic measurements	440
8.8	Future Perspectives	445
9.	Power-to-Fuel and Artificial Photosynthesis for Chemical Energy Storage	493
	<i>Albert Tarancón, Cristian Fábrega, Alex Morata, Marc Torrell, and Teresa Andreu</i>	
9.1	Energy Storage in Current and Future Energy Scenarios	494
9.1.1	Energy Storage Systems	495
9.1.2	Chemical Energy Storage	497
9.1.3	Synthetic Fuels Production	500
9.1.3.1	Fischer-Tropsch synthesis	500
9.1.3.2	Sabatier reaction	501
9.1.4	Efficiency of Converting Chemical Energy into Electricity	502
9.1.4.1	Chemical-to-mechanical-to-electrical conversion: Heat engines	502

9.1.4.2	Direct chemical-to-electrical conversion: Fuel cells	504
9.1.5	One Possible Sustainable Generation/Storage/Consumption Cycle	505
9.2	Power to Fuel	508
9.2.1	General Aspects of Electrolytic Cells	509
9.2.1.1	Fundamentals of electrolysis	509
9.2.1.2	Temperature and pressure effects on electrolysis	511
9.2.1.3	Types of electrolyzers according to the electrolyte	515
9.2.1.4	Non-ideal electrolyzers	517
9.2.1.5	Cell efficiency	520
9.2.2	Electrolysis of Water	520
9.2.2.1	Low-temperature electrolyzers	522
9.2.2.2	High-temperature electrolyzers	529
9.2.3	Coelectrolysis of Water and Carbon Dioxide	536
9.2.3.1	Low-temperature carbon dioxide electrolysis	536
9.2.3.2	High-temperature co-electrolysis of steam and carbon dioxide in SOECs	536
9.2.3.3	Polygeneration in solid oxide fuel cells	539
9.3	Artificial Photosynthesis	540
9.3.1	General Aspects of Artificial Photosynthesis	540
9.3.2	Water Splitting	543
9.3.2.1	Photolysis of water	543
9.3.2.2	Photoelectrochemical water splitting	548
9.3.3	Photoreduction of Carbon Dioxide	551
9.4	Concluding Remarks	555

10. Hydrogen Storage 567*Raphaël Janot*

10.1	Conventional Hydrogen Storages	570
10.1.1	Compressed Gas	570
10.1.2	Liquid Hydrogen	573
10.2	Hydrogen Physisorption	576
10.2.1	Carbon Materials	577
10.2.2	Zeolites	579
10.2.3	Metal-Organic Frameworks	581
10.3	Metal Hydrides	584
10.3.1	Elements	587
10.3.2	AB ₅ Intermetallic Compounds	589
10.3.3	AB ₂ Intermetallic Compounds	590
10.3.4	AB Intermetallic Compounds	592
10.3.5	A ₂ B Intermetallic Compounds	593
10.3.6	Solid Solutions	594
10.4	Complex Hydrides	595
10.4.1	Borohydrides	596
10.4.1.1	Lithium borohydride: LiBH ₄	596
10.4.1.2	Magnesium borohydride	600
10.4.2	Alanates	600
10.4.3	Silanides	603
10.5	Amides and Imides	608
10.5.1	Hydrogenation of Li ₃ N	609
10.5.2	The Li-Mg-N-H System	612
10.5.3	Other Li-Metal-N-H Systems	614
10.6	Ammonia-Borane	617
10.7	Conclusions	622

Part 4: Energy Transmission and Consumption**11. Superconductors 641***Stuart C. Wimbush*

11.1	Introduction	641
------	--------------	-----

11.2	Fundamental Phenomenology of Superconductivity	642
11.2.1	Origin of Lossless Current Transport	643
11.2.2	Limitations on the Superconducting State	644
11.2.3	Flux Penetration and Flux Pinning	645
11.3	Superconducting Materials for Application	648
11.3.1	First Generation BSCCO Wires	648
11.3.2	Second Generation RBCO Tapes	651
11.3.3	MgB ₂ Wires	653
11.3.4	New Materials on the Horizon	655
11.4	Coated Conductor Fabrication	655
11.5	Superconductors for Energy Applications	659
11.5.1	Superconducting Power Cables	660
11.5.2	Superconducting Transformers	665
11.5.3	Superconducting Generators	667
11.5.4	Superconducting Energy Storage Devices	668
11.5.5	Superconducting Fault Current Limiters	670
11.6	Superconductors for Transportation Applications	672
11.6.1	Superconducting Motors	672
11.6.2	Marine Propulsion Systems	673
11.6.3	Magnetically Levitated Trains	674
11.6.4	Electric Aircraft	676
11.6.5	Personal Electric Vehicles	677
11.7	Paradigm-Shifting Energy Technologies	678
11.7.1	Fusion Power	678
11.7.2	Hydrogen Economy	680
11.7.3	Room-Temperature Superconductivity	680
11.8	Other Applications of Superconductors	682
11.9	Cooling	683
11.10	Cost	685
11.11	Summary	687

12. Solid-State Lighting: An Approach to Energy-Efficient Illumination 693

Mariano Perálvarez, Jorge Higuera, Wim Hertog, Óscar Motto, and Josep Carreras

12.1	Properties of Light	693
12.1.1	Introduction	693
12.1.2	The Visual System	695
12.1.3	The Chromaticity Diagram	697
12.1.4	Luminous Efficacy of Radiation	698
12.1.5	Colour Temperature	699
12.1.6	Colour Rendering Index	699
12.1.7	Spectrum and Quality of Light	700
12.2	Light Sources	702
12.2.1	Introduction	702
12.3	LED Physics	705
12.3.1	Semiconductors	705
12.3.1.1	Doping	707
12.3.1.2	p-n junctions	708
12.3.1.3	Direct and indirect band gaps	709
12.3.1.4	LED architecture	710
12.3.1.5	Manufacturing processes	712
12.4	Light Emitting Diodes Based on III-V Junctions	713
12.4.1	Gallium Arsenide	714
12.4.2	Gallium Arsenide Phosphide and Gallium Phosphide	714
12.4.3	Aluminium Gallium Arsenide	715
12.4.4	Aluminium Gallium Indium Phosphide	715
12.4.5	Gallium Nitride and Indium Gallium Nitride	716
12.4.6	ZnSe	717
12.4.7	Materials for UV LEDs	718
12.5	Organic Light Emitting Diodes	718
12.6	White Light with LEDs	721
12.6.1	Wavelength Converters	721

12.6.1.1	Phosphors for LEDs	722
12.6.1.2	Phosphor application methods	723
12.6.2	Multichromatic LED Sources	724
12.6.2.1	Dichromatic LEDs	724
12.6.2.2	Trichromatic LEDs	724
12.6.2.3	Polychromatic LEDs	725
12.6.2.4	Spectral characteristics of multichromatic LED sources	726
12.7	New Approaches	727
12.7.1	Silicon-Based Emitters	727
12.7.2	Quantum Dots	728
12.8	LED Packaging	729
12.8.1	Low-Power LED Packaging	730
12.8.2	Mid- and High-Power LED Packaging	730
12.8.3	Thermal Management	731
12.8.4	Some Effects Related to Excessive Junction Temperature	733
12.8.5	The Role of the Packaging on Light Extraction	734
12.9	LED Drivers	737
12.9.1	Linear Constant-Current Drivers	738
12.9.2	Switching Constant-Current LED Drivers	739
12.9.2.1	Buck converters	740
12.9.2.2	Boost converter	740
12.9.2.3	Boost-buck converter	741
12.10	Lighting Control Systems and Applications	742
12.10.1	Smart Lighting Control Systems	742
12.10.2	Occupancy Sensors	743
12.10.2.1	Illuminance sensors	744
12.10.2.2	Colour sensors	745
12.10.2.3	Spectral sensors	745
12.10.3	Sustainable Energy-Efficient Applications for Smart Cities	746

12.10.3.1	Smart outdoor urban lighting	746
12.10.3.2	Visible light communications	747
12.10.3.3	Adaptive LED lighting	748
12.10.3.4	Indoor spectrally tunable LED luminaires	749
13.	Solid-State Refrigeration Based on Caloric Effects	753
	<i>Seda Aksoy</i>	
13.1	Magnetocaloric Effect	754
13.1.1	Theory of the MCE	754
13.1.2	Magnetocaloric Materials	759
13.1.2.1	Rare earth (lanthanide) elements and their compounds	759
13.1.2.2	3d-transition metal compounds and manganites	761
13.1.3	Refrigeration Technology	764
13.2	Mechanocaloric Effect	768
13.2.1	Mechanocaloric Materials	769
13.2.2	Mechanocaloric Refrigeration	771
13.3	Electrocaloric Effect	772
13.3.1	Electrocaloric Materials	774
13.3.2	Electrocaloric Refrigeration	775
13.4	Conclusion	778
	<i>Index</i>	791

Preface

Materials are fundamental for us humans. Their importance is such that key stages of our civilization have been named after them, each new stage being brought about by a new material that revolutionized existing technologies. Early humans made most of their tools from flint during the Stone Age. The next stages of civilization, from the Copper Age, to the Bronze Age, to the Iron Age, represented a succession of stronger and stronger alloys that led to better tools. More recently, silicon permitted the extraordinary development of modern electronics that profoundly transformed the way we live and communicate. Arguably, the twentieth century was therefore the Age of Silicon, but we must not overlook the myriad of other modern materials that also helped revolutionize our lives. For example, carbon-fiber composites that are light and strong enabled us to fly affordably, and ceramics and metals that are biocompatible allowed us to rebuild ourselves.

With the turn of the century, there are difficult challenges ahead. According to current projections, the world population will reach eight billion by 2030 and will likely reach nine billion by 2050. Such a dramatic increase in population will lead, among other things, to a huge increase in energy demand worldwide. Meeting this ever-increasing demand represents without doubt one of the main challenges of the twenty-first century and will become more and more critical as the fossil fuels on which we rely to generate most of our energy start to run out. It is therefore vital to search for alternative energy sources that are renewable and to find new ways of using energy more efficiently. Any of such new technologies will most likely rely on new materials with outstanding properties, and so the twenty-first century will be perhaps eventually known as the Age of Materials for Energy.

In this context, the purpose of this book is to give a unified and comprehensive presentation of the materials that may underpin this so-needed energy revolution. After a general introduction

(Chapter 1), the book is divided into three blocks that describe materials for energy conversion (Chapters 2–6), energy storage (Chapters 7–10), and energy transmission and consumption (Chapters 11–13). Each chapter is self-contained and includes both fundamentals and latest research results. The book should therefore prove useful for undergraduate and graduate students and researchers working on sustainable energies.

This book would not have happened if it were not for the extraordinary work of all contributing authors, the thorough revision from a selected group of reviewers, and the continuous support from the whole team at Pan Stanford.

Xavier Moya

Cambridge, United Kingdom

David Muñoz-Rojas

Grenoble, France

March 2016